## Metastability, selectivity and molecular transport in gas hydrates : neutron contribution... but not only !

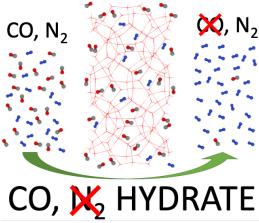
Claire Petuya<sup>a</sup>, Cyrielle Métais<sup>a,b,c</sup>, Ludovic Martin-Gondre<sup>c</sup>, Jacques Ollivier<sup>b</sup>, Françoise Damay<sup>d</sup>, <u>Arnaud Desmedt</u><sup>a\*</sup>

- a. Groupe Spectroscopie Moléculaire, ISM UMR5255 CNRS Univ. Bordeaux
- b. Institut Laue Langevin, Grenoble
- c. UTINAM UMR6213 CNRS Univ Franche-Comté
- d. Laboratoire Léon Brillouin, UMR12 CNRS CEA, Saclay

\* email: arnaud.desmedt@u-bordeaux.fr

The natural occurrence of large quantities of gas hydrates in deep oceans, permafrost and plausibly in extraterrestrial planets or comets, is certainly at the origin of numerous developments and researches in fields ranging from physical-chemistry, geosciences or astrophysics to chemical engineering and innovative technologies. Gas hydrates are ice-like systems made of water molecules forming nano-cages stabilized by the encapsulation of foreign molecules. At a fundamental level, their nanostructuration confers on these materials specific properties (e.g. metastability [1,2], molecular selectivity [3,4], molecular transport [5], etc.) and original formation mechanism. The understanding of their molecular interactions play a key role in the future developments - requiring to combine advanced experimental and theoretical approaches, in which neutron scattering constitutes a unique tool... but not only. The presentation will review recent physico-chemical results relevant in gas hydrates sciences and associated challenges.

- [1] Métais et al, J. Phys. Chem. C 125(11) 6433-6441 (2021)
- [2] Petuya et al, J. Chem. Phys. 150(18) 184705 (2019)
- [3] Petuya et al, J. Phys. Chem. C 122(1) 566 -573 (2018)
- [3] Petuya et Desmedt, J. Phys. Chem. C 123(8) 4871-4878 (2019)
- [4] Petuya et al, Chem. Comm. 54 4290-4293 (2018)
- [2] Nguyen et al, Frontiers in Chemistry 8, 550862 (2020)



**Figure 1:** Representation of the CO selective trapping in the mixed CO-N<sub>2</sub> gas hydrate and of the potential sieving role played by the gas hydrate.